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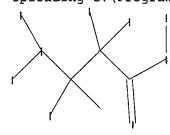
=> ....Testing the current file.... screen

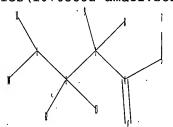
ENTER SCREEN EXPRESSION OR (END):end

=> screen 1006 AND 2076

L1 SCREEN CREATED

Uploading C:\Program Files\Stnexp\Queries\10765832 amdt1.str





chain nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13

chain bonds :

1-2 1-10 1-11 2-3 2-12 2-13 3-4 3-8 3-9 4-5 4-6 5-7

exact/norm bonds :

1-2

exact bonds :

1-10 1-11 2-3 2-12 2-13 3-4 3-8 3-9 5-7

normalized bonds :

4-5 4-6

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom

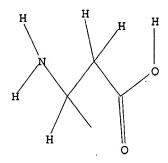
=> que L2 AND L1

L3 QUE L2 AND L1

=> d L2

L2 HAS NO ANSWERS

L2 · STR



Structure attributes must be viewed using STN Express query preparation.

=> s L2 full FULL SEARCH INITIATED 09:43:29 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 853388 TO ITERATE

100.0% PROCESSED 853388 ITERATIONS

38540 ANSWERS

SEARCH TIME: 00.00.06

L4 38540 SEA SSS FUL L2

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 172.10 172.31

FULL ESTIMATED COST

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FILE COVERS 1907 - 20 Jun 2007 VOL 146 ISS 26 FILE LAST UPDATED: 19 Jun 2007 (20070619/ED)

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```
L5
         78672 L4
=> s optically active
        101622 OPTICALLY
        984736 ACTIVE
          1209 ACTIVES
        985434 ACTIVE
                  (ACTIVE OR ACTIVES)
         39040 OPTICALLY ACTIVE
L6
                  (OPTICALLY (W) ACTIVE)
=> s L5 and L6
           268 L5 AND L6
L7
=> s lithium amide
        325570 LITHIUM
           370 LITHIUMS
        325698 LITHIUM
                  (LITHIUM OR LITHIUMS)
        130526 AMIDE
         82074 AMIDES
        177948 AMIDE
                  (AMIDE OR AMIDES)
L8
          1486 LITHIUM AMIDE
                  (LITHIUM(W)AMIDE)
=> s L7 and L8
L9
             1 L7 AND L8
=> d L9 bib abs
     ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
     1990:424454 CAPLUS
DN
     113:24454
ΤI
     Non-proteinogenic amino acid synthesis. The \beta-anion derived from
     aspartic acid, and its application to \alpha-amino acid synthesis
ΑU
     Baldwin, Jack E.; Moloney, Mark G.; North, Michael
     Dyson Perrins Lab., Univ. Oxford, Oxford, OX1 3QY, UK
CS
     Tetrahedron (1989), 45(19), 6309-18
SO
    CODEN: TETRAB; ISSN: 0040-4020
DT
     Journal
     English
LA
OS
     CASREACT 113:24454
AB
     Treatment of PhCH2O2C-Asp(OMe)-OCMe3 (I) with lithium
     amide bases generates the corresponding \beta-ester enolate,
     which can be alkylated with suitable electrophiles. The application of
     this strategy for synthesis of optically active amino
     acids has been investigated. Thus, treatment of I with LiN(SiMe3)2,
     followed by alkylation with PhCH2Br gave PhCH2O2CNHCH(CO2CMe3)CH(CO2Me)CH2
     Ph (II). Saponification, decarboxylation, and deblocking of II gave
     (S)-homophenylalanine in 80% enantiomeric excess.
=> s alpha beta unsaturated esters
       1692654 ALPHA
          2493 ALPHAS
       1692761 ALPHA
                  (ALPHA OR ALPHAS)
```

1460247 BETA 1325 BETAS 1460324 BETA

> 56941 UNSATURATED 1 UNSATURATEDS 56942 UNSATURATED

(BETA OR BETAS)

```
(UNSATURATED OR UNSATURATEDS)
        228107 UNSATD
             13 UNSATDS
        228110 UNSATD
                  (UNSATD OR UNSATDS)
        243007 UNSATURATED
                  (UNSATURATED OR UNSATD)
        442286 ESTERS
              2 ESTERSES
        442287 ESTERS
                  (ESTERS OR ESTERSES)
L10
           1805 ALPHA BETA UNSATURATED ESTERS
                  (ALPHA (W) BETA (W) UNSATURATED (W) ESTERS)
=> s L8 and L10
L11
            17 L8 AND L10
=> s beta amino acid
       1460247 BETA
           1325 BETAS
       1460324 BETA
                  (BETA OR BETAS)
       1122672 AMINO
             44 AMINOS
       1122690 AMINO
                  (AMINO OR AMINOS)
       4388668 ACID
       1578656 ACIDS
       4888060 ACID
                  (ACID OR ACIDS)
          2949 BETA AMINO ACID
L12
                  (BETA (W) AMINO (W) ACID)
=> s L11 and L12
              9 L11 AND L12
=> d L13 1-9 bib abs
     ANSWER 1 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
     2006:780658 CAPLUS
AN
DΝ
     145:397754
ΤI
     Homochiral lithium amides for the asymmetric synthesis
     of \beta -amino acids
AU
     Davies, Stephen G.; Garrido, Narciso M.; Kruchinin, Dennis; Ichihara,
     Osamu; Kotchie, Luke J.; Price, Paul D.; Mortimer, Anne J. Price; Russell,
     Angela J.; Smith, Andrew D.
     Department of Organic Chemistry, Chemistry Research Laboratory, University
CS
     of Oxford, Oxford, OX1 3TA, UK
SO
     Tetrahedron: Asymmetry (2006), 17(12), 1793-1811
     CODEN: TASYE3; ISSN: 0957-4166
PB
     Elsevier B.V.
DT
     Journal
LΑ
     English
     Secondary homochiral lithium amides derived from
AΒ
     \alpha-methylbenzylamine undergo highly diastereoselective conjugate
     addns. to a range of \alpha , \beta -unsatd.
     esters. The corresponding \beta -amino
     acids are readily liberated by successive N-debenzylation and
     ester hydrolysis, furnishing (R)-\beta-amino butyric acid,
     (R)-\beta-amino pentanoic acid, (S)-\beta-leucine, (R)-\beta-amino
     octanoic acid, (S)-\beta-phenylalanine, (S)-\beta-tyrosine Me ether,
     (S)-\beta-tyrosine hydrochloride and (S)-\beta-(2-methoxyphenyl)-\beta-
     amino propanoic acid in high yields and high ee. The application of this
     procedure to the synthesis of the natural products (R)-\beta-DOPA and
     (R)-\beta-lysine is demonstrated. The development of a simplified
```

one-pot reaction protocol applicable to the multi-gram scale synthesis of homochiral  $\beta$ -amino esters is also delineated.

RE.CNT 89 THERE ARE 89 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L13 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
```

AN 2005:246002 CAPLUS

DN 142:482282

TI Cyclic  $\beta$  -amino acid derivatives: synthesis via lithium amide promoted tandem asymmetric conjugate addition-cyclization reactions

AU Davies, Stephen G.; Diez, David; Dominguez, Sara H.; Garrido, Narciso M.; Kruchinin, Dennis; Price, Paul D.; Smith, Andrew D.

CS Department of Organic Chemistry, Chemical Research Laboratory, University of Oxford, Oxford, OX1 3TA, UK

SO Organic & Biomolecular Chemistry (2005), 3(7), 1284-1301 CODEN: OBCRAK; ISSN: 1477-0520

PB Royal Society of Chemistry

DT Journal

LA English

OS CASREACT 142:482282

AB The product distribution upon conjugate addition of homochiral lithium N-benzyl-N- $\alpha$ -methylbenzylamide to dimethyl-(E,E)-nona-2,7-dienedioate can be controlled to give either the cyclic 1,2-anti-1,6-anti- $\beta$ -amino ester (derived from conjugate addition and intramol. enolate cyclization) or the acyclic bis- $\beta$ -amino ester derivative (derived from double conjugate addition) in high de. The introduction

of a protected nitrogen functionality into the diester skeleton facilitates, after conjugate addition and intramol. enolate cyclization, the asym. construction of piperidines in high de; variation in the N-protecting group indicates that the highest stereoselectivity is observed with  $\alpha$ -branched N-substituents. Tandem conjugate addition-aldol reactions can also be achieved stereoselectively, with lithium amide conjugate addition to .vepsiln.- and  $\zeta$ -oxo- .alpha ., $\beta$ -unsatd. esters giving the corresponding five and six membered cyclic  $\beta$ -amino esters in high de. N-deprotection by hydrogenolysis of the products arising from these reactions furnishes a range of polyfunctionalised transpentacin and

transhexacin derivs. in high de and ee.

RE.CNT 81 THERE ARE 81 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L13 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
```

AN 2004:763180 CAPLUS

DN 141:395393

TI Asymmetric synthesis of 3,4,5,6-tetrasubstituted piperidin-2-ones by three-component coupling

AU Davies, Stephen G.; Smith, Andrew D.; Cowley, Andrew R.

CS Department of Organic Chemistry, Chemistry Research Laboratory, University of Oxford, Oxford, OX1 3TA, UK

SO Synlett (2004), (11), 1957-1960 CODEN: SYNLES; ISSN: 0936-5214

PB Georg Thieme Verlag

DT Journal

LA English

OS CASREACT 141:395393

AB The asym. three-component coupling of  $\alpha$ ,  $\beta$  - unsatd. esters and alkylidenemalonates initiated with a homochiral lithium amide proceeds with high levels of diastereoselectivity, with hydrogenation of the resultant  $\alpha$ -substituted  $\beta$  -amino acid derivs. giving a range of differentially protected 3,4,5,6-

tetrasubstituted piperidinones with four contiguous stereogenic centers.

RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD

## ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN 2002:526645 ANCAPLUS DN 137:295209 TI Ring closing metathesis for the asymmetric synthesis of (S)-homopipecolic acid, (S)-homoproline and (S)-coniine Davies, Stephen G.; Iwamoto, Keiji; Smethurst, Christian A. P.; Smith, ΑU Andrew D.; Rodriguez-Solla, Humberto CS The Dyson Perrins Laboratory, University of Oxford, Oxford, OX1 3QY, UK Synlett (2002), (7), 1146-1148 CODEN: SYNLES; ISSN: 0936-5214 SO PB Georg Thieme Verlag DTJournal English LA OS CASREACT 137:295209 Diastereoselective conjugate addition of lithium (S)-N-allyl-N- $\alpha$ -AB ' methylbenzylamide to  $\alpha$  ,  $\beta$  -unsatd. esters or Weinreb amides, followed by ring closing metathesis is used to afford the cyclic  $\beta$  -amino acids (S)-homopipecolic acid and (S)-homoproline and the amine (S)-coniine in high ee. RE.CNT 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT L13 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN 2002:407900 CAPLUS NΑ DN 137:370329 Asymmetric synthesis of homochiral differentially protected bis-. TI beta.-amino acid scaffolds Bull, Steven D.; Davies, Stephen G.; Roberts, Paul M.; Savory, Edward D.; ΑU Smith, Andrew D. University of Oxford, The Dyson Perrins Laboratory, Oxford, OX1 3QY, UK CS Tetrahedron (2002), 58(23), 4629-4642 SO CODEN: TETRAB; ISSN: 0040-4020 Elsevier Science Ltd. PBDT Journal English LΑ os CASREACT 137:370329 AB A strategy for the asym. synthesis of homochiral [(R,R)- or (S,S)-], or meso-(R,S) bis- $\beta$  -amino acid scaffolds, formally resulting from the stepwise conjugate addition of two differentially protected homochiral lithium amides to two . alpha.,β -unsatd. esters attached to a central arene, is demonstrated. Further manipulation enables the efficient synthesis of orthogonally protected pseudo-meso or pseudo-C2 sym. scaffolds via selective N-benzyl or N-allyl deprotection, enabling regio-, stereo- and chemoselective functionalization. THERE ARE 88 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 88 ALL CITATIONS AVAILABLE IN THE RE FORMAT L13 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN ΑN 2000:282509 CAPLUS DN 133:89282 A chiral, oxidatively cleavable auxiliary in conjugate additions of lithium amides. Preparation of enantiomerically pure . beta.-amino acid derivatives ΑU Podlech, Joachim Institut fur Organische Chemie der Universitat Stuttgart, Stuttgart, CS D-70569, Germany Synthetic Communications (2000), 30(10), 1779-1786 SO CODEN: SYNCAV; ISSN: 0039-7911

PB

DT

LA

Marcel Dekker, Inc.

Journal

English

AB Addition of the lithium salts of enantiomerically pure α-methyl-4-methoxybenzylamines I (R = allyl, 4-MeOC6H4CH2) to α ,.
beta.-unsatd. esters R1CH:CHCO2R2 (R1, R2 = Ph, tert-Bu; Ph, Me; Me, Et) gave β -amino
acid derivs. II with stereoselectivities > 95:5. The chiral
auxiliary in II (R = 4-MeOC6H4CH2; R1 = Ph; R2 = Me) was cleaved by oxidation with cerium(IV) ammonium nitrate and subsequent hydrolysis of the resulting imines to give (S)-PhCH(NH2)CH2CO2Me in 60% yield.

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1998:619258 CAPLUS

DN 130:4037

TI Tandem protocol for the stereoselective synthesis of different polyfunctional  $\beta$  -amino acids and 3-amino-substituted carbohydrates

AU Sewald, Norbert; Hiller, Klaus D.; Koerner, Matthias; Findeisen, Matthias

CS Department of Organic Chemistry, University of Leipzig, Leipzig, Germany

SO Journal of Organic Chemistry (1998), 63(21), 7263-7274 CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

GΙ

$$R^{1}$$
 $CO_{2}R^{2}$ 
 $R^{3}$ 
 $CO_{2}R^{2}$ 
 $R^{3}$ 
 $R^{3}$ 
 $CO_{2}R^{2}$ 

AB Conjugate addition of homochiral amidocuprates or lithium amides derived from (R)-N-(1-phenylethyl) (trimethylsilyl)amine to  $\alpha$  ,  $\beta$  -unsatd. esters, (E)-R1CH:CHCO2R2 (R1 = Me, Et, CHMe2, Ph; R2 = Et, Me), proceeds stereoselectively and allows the synthesis of  $\beta$  -amino acids I (R3 = H). Trapping of the intermediate ester enolate with D2O affords the corresponding deuterated compds. I (R3 = D). Anti- $\alpha$ -alkyl- $\beta$ -amino acids are obtained stereoselectively after transmetalation of the lithium/copper ester enolate to the titanium ester enolate and trapping with carbon electrophiles. Both diastereomers of  $\beta$ -homothreonine, other precursors of 3-amino-substituted carbohydrates, and stereoselectively

deuterated analogs at position 2 are formed from enantiomerically pure  $\gamma$ -alkoxy-substituted enoates. The product distribution observed is complementary to published results regarding 1,4-addition to  $\gamma$ -silyloxy-substituted enoates. The anti/syn selectivity can be explained by assuming transition state geometries where the delivery of the nitrogen nucleophile is controlled by lithium "chelation" between reagent and substrate. In one case the product configuration can be controlled by the reagent irresp. of the substrate stereochem.; in other cases, the topicity of the addition is complementary to published results. For instance, erythro- or threo-configured 2,3-dideoxy-3-aminopentoses are accessible via this route.

RE.CNT 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L13 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
- AN 1997:692754 CAPLUS
- DN 127:331307
- TI  $(1's,4s)-2-aryl-4-(1'-hydroxybenzyl)-4,5-dihydrooxazole as a useful chiral auxiliary for the synthesis of <math>\beta$ -amino acids and  $\beta$ -lactams in a highly stereoselective manner
- AU Shimizu, Makoto; Maruyama, Shingo; Suzuki, Yasuhiro; Fujisawa, Tamotsu
- CS Dep. Chem. Materials, Mie Univ., Mie, 514, Japan
- SO Heterocycles (1997), 45(10), 1883-1889 CODEN: HTCYAM; ISSN: 0385-5414
- PB Japan Institute of Heterocyclic Chemistry
- DT Journal
- LA English
- OS CASREACT 127:331307
- AB (1'S,4S)-2-Aryl-4-(1'-hydroxybenzyl)-4,5-dihydroxazole prepared from (1S,2S)-2-amino--1-phenylpropane-1,3-diol has been found to be a useful chiral auxiliary from the stereoselective synthesis of  $\beta$ -lactams and  $\beta$ -amino acids in the reaction of imine-ester enolate condensation or 1,4-addition of lithium amides to  $\alpha$ ,  $\beta$ -unsatd. esters.
- RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L13 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
- AN 1991:429864 CAPLUS
- DN 115:29864
- TI Asymmetric synthesis of R- $\beta$ -aminobutanoic acid and S- $\beta$ -tyrosine: homochiral lithium amide equivalents for Michael additions to  $\alpha$  ,  $\beta$  -unsaturated esters
- AU Davies, Stephen G.; Ichihara, Osamu
- CS Dyson Perrins Lab., Univ. Oxford, Oxford, OX1 3QY, UK
- SO Tetrahedron: Asymmetry (1991), 2(3), 183-6 CODEN: TASYE3; ISSN: 0957-4166
- DT Journal
- LA English
- OS CASREACT 115:29864
- AB Michael addition of (R)-PhCHMeNLiCH2Ph to (E)-MeCH:CHCO2CH2Ph is highly stereoselective (95% diastereomeric excess), giving after debenzylation and crystallization homochiral (R)- $\beta$ -aminobutanoic acid. A similar addition to
  - (E)-4-PhCH2OC6H4CH:CHCO2Me is completely stereoselective giving after debenzylation and acid hydrolysis homochiral (S)- $\beta$ -tyrosine as its HCl salt.

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http://www.cas.org/support/stngen/stndoc/properties.html

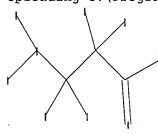
=> ....Testing the current file.... screen

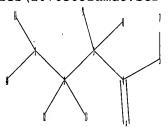
ENTER SCREEN EXPRESSION OR (END):end

=> screen 1006 AND 2076

L1 SCREEN CREATED

Uploading C:\Program Files\Stnexp\Queries\10765832amdt.str





chain nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13

chain bonds :

1-2 1-10 1-11 2-3 2-12 2-13 3-4 3-8 3-9 4-5 4-6 5-7

exact/norm bonds :

1-2 2-13

exact bonds :

1-10 1-11 2-3 2-12 3-4 3-8 3-9 5-7

normalized bonds :

4-5 4-6

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom

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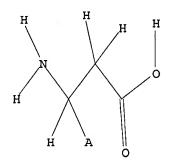
=> que L2 AND L1

L3 QUE L2 AND L1

=> d L2

L2 HAS NO ANSWERS

L2 STR



Structure attributes must be viewed using STN Express query preparation.

=> s L2 full

FULL SEARCH INITIATED 09:13:43 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 943166 TO ITERATE

100.0% PROCESSED 943166 ITERATIONS

38585 ANSWERS

SEARCH TIME: 00.00.06

L4 38585 SEA SSS FUL L2

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 172.10 172.31

FULL ESTIMATED COST

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```
L5
         78721 L4
=> s process
       2445141 PROCESS
       1661071 PROCESSES
L6
       3644695 PROCESS
                · (PROCESS OR PROCESSES)
=> s L5 and L6
L7
          6269 L5 AND L6
=> s beta amino acids
       1460247 BETA
          1325 BETAS
       1460324 BETA
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       1122672 AMINO
            44, AMINOS
       1122690 AMINO
                 (AMINO OR AMINOS)
       1578656 ACIDS
rs
          1611 BETA AMINO ACIDS
                 (BETA (W) AMINO (W) ACIDS)
=> s L7 and L8
            17 L7 AND L8
=> d L9 1-17 bib abs hitstr
L9
     ANSWER 1 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN
ΑN
     2007:385362 CAPLUS
DN
     146:396162
TI
     Recombinantly produced polyhydroxyalkanoate polymer particles displaying
     fusion proteins for a variety of diagnostic, analytical, and therapeutic
IN
     Rehm, Bernd Helmut Adam; Backstrom, Bjorn Thomas
PA
     N.Z.
SO
     PCT Int. Appl., 199pp.
     CODEN: PIXXD2
DT
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LA
     English
FAN.CNT 1
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                                            APPLICATION NO.
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PΙ
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                                                                    20060927
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             KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN,
             MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS,
             RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
PRAI NZ 2005-542644
                                20050927
                          Α
     NZ 2005-544096
                          Α
                                20051212
     NZ 2005-544097
                          Α
                                20051212
     The present invention relates to production and use of polymer particles where
AB
     the polymer comprises poly(\beta -amino acids
     ), polylactates, polythioesters, or polyesters, and in particular
     polyhydroxyalkanoates (PHA) or more specifically poly(3-hydroxybutyrate).
     In particular the invention relates to functionalized polymer particles,
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processes of production, and uses thereof. Production of polymer particles are produced by recombinant host cells transfected with expression constructs comprising at lease one nucleotide sequence encoding a polymer synthase and at least one nucleotide sequence encoding a fusion protein of polymer synthase and at least one fusion partner, and optionally addnl. fusions of polymer particle-binding domains and a fusion partner. The method is exemplified by the preparation of PHA particles displaying fusion polypeptides comprising phasin (PhaP from Ralstonia eutropha) and mouse oligodendrocyte glycoprotein (MOG) or interleukin-2, or a fusion polypeptide comprising an antibody binding the ZZ domain of Staphylococcus aureus protein A. The methods, polymer particles and fusion proteins of the present invention have utility in diagnostics, protein production, biocatalyst immobilization, and drug delivery.

IT 98849-88-8, FLAG peptide

RL: BUU (Biological use, unclassified); NUU (Other use, unclassified); BIOL (Biological study); USES (Uses)

(fusion partner on polymer particles; recombinantly produced polyhydroxyalkanoate polymer particles displaying fusion proteins for a variety of diagnostic, anal., and therapeutic uses)

98849-88-8 CAPLUS RN

CN L-Lysine, L-α-aspartyl-L-tyrosyl-L-lysyl-L-α-aspartyl-L- $\alpha$ -aspartyl-L- $\alpha$ -aspartyl- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

```
2006:1007676 CAPLUS
AN
DN
     145:376924
     Improved process for preparation of optically pure substituted
     \beta-amino heptanoic acids as ligands for \alpha-2\delta-subunit of
     calcium channel for treatment of pain and sleep disorders
     Franczyk, Thaddeus Stephan, II; Herrinton, Paul Matthew; Perrault, William
IN
     Roland
PΑ
     Pharmacia & Upjohn Company LLC, USA
     PCT Int. Appl., 74pp.
SO
     CODEN: PIXXD2
DΤ
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                   DATE
     ______
                               . _ _ _ _ _ _ _ _
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PΙ
     WO 2006100568
                              20060928 WO 2006-IB637
                         A1
                                                                   20060313
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR,
             KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
             MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
             SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
             VN, YU, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
     JP 2006265251
                          Α
                                20061005
                                            JP 2006-80221
                                                                    20060323
PRAI US 2005-665502P
                          Ρ
                                20050324
     MARPAT 145:376924
     Non-racemic 3-amino-4-R1-5-R2-7-R3-heptanoic acids, having at least 2
AB
     stereogenic centers (1, R1, R2, R3 = H, C1-6 alkyl, C3-6 cycloalkyl, aryl,
     aralkyl, arylamino, optionally substituted with Cl, F, NH2, NO2, CN
     groups; C1-3 alkyl optionally F1-3-substituted; R1 and R2 \neq H),
     useful as ligands for calcium channel for treatment of pain and sleep
     disorders, including insomnia, fibromyalgia, epilepsy, neuropathic pain
     and others (no data), were prepared by an improved process
     comprising asym. hydrogenation of dienoic R6-esters of
     3-(R7-amino)-4-R1-5-R2-7-R3-2,6-heptanedioic acids (6; same R1, R2, R3; R6
     = H, optionally unsatd. C1-7 organyl; R7 = H, C1-7 acyl) with subsequent
     optional hydrolysis. The compds. 6 were prepared by stereoselective addition
     of allylamines R2CH:CHCH(R3)NR4R5 [2, preferably having (1R,2Z)- or
     (1S, 2E) -configuration; R4, R5 = C1-6 alkyl, preferably R4R5N =
     (S)-2-methyl-1-pyrrolidinyl] with 2-butynoates R1CH2C.tplbond.CCOOR6 (same
     R1, R6) in the presence of Lewis bases, preferably Et3N, or Lewis acids,
     preferably Group IA-Group IIIA metal salts, to give the tertiary enamines,
     3-(R4R5-amino)-4-R1-5-R2-7-R3-2,6-heptanedioic acids (5, same R), followed
     by conversion of 5 to 6 by reaction with ammonia. In an example, Et
     (3S,5R)-3-acetylamino-5-methyloctanoate was prepared by asym. hydrogenation
     of 4.179 mmol of Et (2Z,5S,6E)-3-acetylamino-5-methyl-2,6-octadienoate in
     the presence of 0.042 mmol of [[(R)-BINAPINE](NBD)Rh]BF4 in 15 mL of MeOH
     at 2 atm of H2 and 30° for 26 h, followed by hydrogenation on 0.5 g
     of 5% Pd/C at 2 atm and 30° for 18 h; the ester was then hydrolyzed
     affording (3S,5R)-1 (R1 = H, R2 = R3 = Me) with 92% yield and 96.3% of
     diastereomeric purity.
IT
     610300-00-0P 866108-39-6P 866108-50-1P
     911053-42-4P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (process for preparation of chiral β-amino heptanoic acids as
        ligands for \alpha-2\delta-subunit of calcium channel for treatment
        of pain and sleep disorders)
RN
     610300-00-0 CAPLUS
CN
     Octanoic acid, 3-amino-5-methyl-, hydrochloride, (3S,5R)- (9CI)
```

ANSWER 2 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN

L9

NAME)

Absolute stereochemistry. Rotation (-).

HCl

RN 866108-39-6 CAPLUS

CN Octanoic acid, 3-amino-4,5-dimethyl-, hydrochloride, (3R,4R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

HCl

RN 866108-50-1 CAPLUS

CN Heptanoic acid, 3-amino-4,5-dimethyl-, hydrochloride, (3R,4R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

HCl

RN 911053-42-4 CAPLUS

CN Octanoic acid, 3-amino-5-methyl-, hydrochloride, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

## RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT ANSWER 3 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN L9AN2005:215641 CAPLUS DN 142:261785 TI Process for obtaining enantiopure compounds Callens, Roland; Blondeel, Georges; Pousset, Cyrille; Gire, Ronan IN PA Solvay Sa, Belg. Fr. Demande, 20 pp. so CODEN: FRXXBL DT Patent LΑ French FAN.CNT 1 PATENT NO. KIND DATE APPLICATION NO. DATE -------------------PI FR 2859471 A1 20050311 FR 2003-10582 20030909 FR 2859471 B1 20060203 WO 2005023838 A1 20050317 WO 2004-EP52094 20040908 AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG EP 1664084 20060607 EP 2004-766744 20040908 Α1 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC; PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK CN 1845934 20061011 CN 2004-80025613 20040908 Α US 2007027326 A1 20070201 US 2006-570933 20060308 PRAI FR 2003-10582 20030909 Α WO 2004-EP52094 W 20040908 CASREACT 142:261785 OS The invention relates to a process for obtaining enantiopure .AB compds. which have at least one functional group which can react with an activated carboxyl group. Specifically, the method can be applied to the separation of enantiomers of a $\beta$ -amino acid by reaction with an

compds. which have at least one functional group which can react with an activated carboxyl group. Specifically, the method can be applied to the separation of enantiomers of a  $\beta$ -amino acid by reaction with an N-protected  $\alpha$ -amino acid activated derivative. Thus, treatment of persilylated DL-3-amino-3-phenylpropionic acid with 1-tosyl-L-pyroglutamyl chloride in AcOEt in the presence of Et3N afforded dipeptide product as a mixture of diastereomers. Chromatog. separation of the diastereomers and treatment with 4 N HCl yielded D-3-amino-3-phenylpropionic acid, along with N-tosyl-L-glutamic acid.

IT 541-48-0

RL: RCT (Reactant); RACT (Reactant or reagent) (process for obtaining enantiopure  $\beta$  - amino acids)

RN 541-48-0 CAPLUS

CN Butanoic acid, 3-amino- (CA INDEX NAME)

 $\begin{array}{c} ^{\rm NH_2} \\ | \\ ^{\rm Me-CH-CH_2-CO_2H} \end{array}$ 

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 4 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN
ΑN
     2005:36482 CAPLUS
DN
     142:133207
     Enzymic stereospecific and enantiomeric enrichment of \beta -
TI
     amino acids
     Chase, Matthew; Clayton, Robert; Landis, Bryan; Banerjee, Amit
IN
PA
     Pharmacia Corporation, USA
SO
     U.S. Pat. Appl. Publ., 44 pp.
     CODEN: USXXCO
DT
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                    DATE
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                                            ______
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PI
     US 2005009151
                         A1
                                20050113
                                            US 2004-875161
                                                                   20040622
     CA 2529509
                         A1
                                20050120
                                            CA 2004-2529509
                                                                    20040630 -
     WO 2005005633
                         A2
                                20050120
                                            WO 2004-IB2183
                                                                    20040630
     WO 2005005633
                         A3
                                20050512
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
             SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
             SN, TD, TG
     EP 1646718
                          A2
                                20060419
                                            EP 2004-743849
                                                                    20040630
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK
                                            BR 2004-12308
     BR 2004012308
                          Α
                                20060620
                                                                    20040630
PRAI US 2003-486032P
                          Р
                                20030710
     US 2003-499622P
                          Р
                                20030902
     WO 2004-IB2183
                          W
                                20040630
OS
     MARPAT 142:133207
     The present invention relates to methods for the stereospecific synthesis
AB
     and for the enantiomeric enrichment of \boldsymbol{\beta} -amino
     acids. A novel D-\beta-aminotransferase, which exhibits
     stereoselectivity for D-\beta-phenylalanine, (D-3-amino-3-phenylpropinine
     acid) was purified from a newly-isolated strain of Variouorax paradoxus.
    A novel L-\beta-aminotransferase was purified from a newly-isolated
     strain of Alcaligenes eutrophus . The D- and L-\beta-aminotransferases
     can be used to facilitate the stereoselective biosynthesis of
     \beta-D-phenylalanine or \beta-L-phenylalanine, from a mixture of
     L-glutamic acid or L-alanine, resp., and 3-keto-3-phenylpropionic acid in
     the presence of the cofactor pyridoxal phosphate.
IT
     541-48-0P, 3-Aminobutyric acid 3653-34-7P
     18664-78-3P, 3-Aminopentanoic acid 150618-42-1P
     824424-63-7P 824424-67-1P 824424-68-2P
     824424-70-6P 824424-72-8P
     RL: BCP (Biochemical process); BPN (Biosynthetic preparation); RCT
     (Reactant); BIOL (Biological study); PREP (Preparation); PROC (Process);
     RACT (Reactant or reagent)
        (enzymic stereospecific and enantiomeric enrichment of \beta
        -amino acids)
     541-48-0 CAPLUS
RN
CN
     Butanoic acid, 3-amino- (CA INDEX NAME)
```

L9

RN 3653-34-7 CAPLUS CN Hexanoic acid, 3-amino-5-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

 $\begin{array}{c} \text{NH}_2 \\ | \\ \text{HO}_2\text{C--} \text{CH}_2\text{--} \text{CH--} \text{Bu-i} \end{array}$ 

RN 18664-78-3 CAPLUS

CN Pentanoic acid, 3-amino- (9CI) (CA INDEX NAME)

 $\begin{array}{c} \mathrm{NH_2} \\ | \\ \mathrm{Et-CH-CH_2-CO_2H} \end{array}$ 

RN 150618-42-1 CAPLUS

CN Hexanoic acid, 3-amino-4,4,5,5,6,6,6-heptafluoro- (9CI) (CA INDEX NAME)

 $\begin{array}{c} \mathrm{NH_2} \\ | \\ \mathrm{HO_2C-CH_2-CH-CF_2-CF_2-CF_3} \end{array}$ 

RN 824424-63-7 CAPLUS

CN Cyclopentanepentanoic acid,  $\beta$ -amino- (9CI) (CA INDEX NAME)

RN 824424-67-1 CAPLUS

CN Pentanoic acid, 3-amino-5-chloro-4,4-dimethyl- (9CI) (CA INDEX NAME)

RN 824424-68-2 CAPLUS

CN Propanoic acid, 3-amino-3-(methylthio)- (9CI) (CA INDEX NAME)

 $\begin{array}{c} \text{SMe} \\ | \\ \text{H}_2\text{N--} \text{CH---} \text{CH}_2\text{---} \text{CO}_2\text{H} \end{array}$ 

RN 824424-70-6 CAPLUS

CN Propanoic acid, 3-amino-3-(4-chlorobutoxy)- (9CI) (CA INDEX NAME)

```
NHo
Cl-(CH_2)_4-O-CH-CH_2-CO_2H
RN
     824424-72-8 CAPLUS
     Butanoic acid, 3-amino-4-methoxy- (9CI) (CA INDEX NAME)
CN
         NH_2
MeO-CH_2-CH-CH_2-CO_2H
     5427-96-3P, 3-Aminoadipic acid
IT
     RL: BCP (Biochemical process); BYP (Byproduct); RCT (Reactant); BIOL
     (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or
        (enzymic stereospecific and enantiomeric enrichment of \beta
        -amino acids)
RN
     5427-96-3 CAPLUS
     Hexanedioic acid, 3-amino- (7CI, 8CI, 9CI) (CA INDEX NAME)
CN
          NH<sub>2</sub>
HO_2C-CH_2-CH-CH_2-CH_2-CO_2H
IT
     5699-54-7
     RL: BCP (Biochemical process); RCT (Reactant); BIOL (Biological study);
     PROC (Process); RACT (Reactant or reagent)
        (enzymic stereospecific and enantiomeric enrichment of \beta
        -amino acids)
RN
     5699-54-7 CAPLUS
     Pentanoic acid, 3-amino-4-methyl-
                                         (CA INDEX NAME)
CN
     NH_2
i-Pr-CH-CH2-CO2H
    58521-63-4P, 3-Aminohexanoic acid
IT
     RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP
     (Preparation)
        (enzymic stereospecific and enantiomeric enrichment of \beta
        -amino acids)
RN
     58521-63-4 CAPLUS
     Hexanoic acid, 3-amino- (7CI, 9CI)
                                          (CA INDEX NAME)
CN
     NH_2
n-Pr-CH-CH2-CO2H
IT
     147228-37-3 218278-62-7
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (enzymic stereospecific and enantiomeric enrichment of \beta
        -amino acids)
RN
     147228-37-3 CAPLUS
     Benzenepentanoic acid, \beta-amino-, (\betaR)- (9CI) (CA INDEX NAME)
CN
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Absolute stereochemistry.

RN 218278-62-7 CAPLUS

CN Benzenepentanoic acid,  $\beta$ -amino-, ( $\beta$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry:

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ANSWER 5 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN
L9
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AN2003:473144 CAPLUS

DN 139:51694

ΤI Methods for the preparation of  $\beta$  -amino

IN Frey, Perry A.; Ruzicka, Frank J.

PA Wisconsin Alumni Research Foundation, USA

U.S. Pat. Appl. Publ., 34 pp., Cont.-in-part of U.S. Ser. No. 847,010. CODEN: USXXCO

DT Patent

LA English

FAN.	-																	
		ENT 1	NO.			KIN		DATE								D	ATE	
ΡI	US	2003	11388	32				2003	0619		US 20					2	0020	905
		6248						2001	0619	1	US 19	999-	3306	ıi 🗀		1:	9990	611
	US 2002173637			A1		20021121		,	US 2001-847010					20010501				
	WO 2004021981			A2 20040318			WO 2003-US27235					20030829						
	WO	2004	02198	31		A3		2005	0602									
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
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			GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,
			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	ΝZ,	· OM,
			PG,	PH,	ΡL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	TJ,	TM,	TN,
•			TR,	TT,	TZ,	UA,	ŪĠ,	UΖ,	VC,	VN,	YU,	ZA,	ZM,	ZW				
		RW:	GH,	GM,	ΚE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,
			KG,	ΚZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	ĊY,	CZ,	DE,	DK,	EE,	ES,
			FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	TR,
			BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG
AU 2003265845			A1		20040329 AU 2003-265845						20030829							
PRAI	PRAI US 1998-198942			B2										,				
	US	1999	-3306	511		A3		1999	0611									
		2001						2001	0501									
		2002						2002	-									
		2003						2003	0829								•	
OS	CDC	יים ביו קו	ጥ ገገሩ	9 - 51	694													

os CASREACT 139:51694

AB Purified  $\beta$  -amino acids are of

considerable interest in the preparation of pharmacol. active compds. and industrial precursors. Although enantiomerically pure  $\beta$  amino acids can be produced by standard chemical synthesis, this traditional approach is time consuming, requires expensive starting materials, and results in a racemic mixture which must be purified further. However, DNA mols. encoding lysine 2,3-aminomutase can be used to prepare . beta.-amino acids by methods that avoid the pitfalls of chemical synthesis. The present invention provides a method of producing enantiomerically pure  $\beta$  -amino acids from  $\beta$  -amino acids comprising catalyzing the conversion of an  $\beta$ -amino acid to a corresponding  $\beta$ -amino acid by utilizing a lysine 2,3-aminomutase as the catalyst.

IT 504-21-2P, L- $\beta$ -Lysine

RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation) (methods for the preparation of  $\beta$  -amino acids)

RN 504-21-2 CAPLUS

CN Hexanoic acid, 3,6-diamino-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L9 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2002:116693 CAPLUS

DN 136:295053

TI Reactivity of Amino Acids in Nitrosation Reactions and Its Relation to the Alkylating Potential of Their Products

AU Garcia-Santos, M. Del Pilar; Gonzalez-Mancebo, Samuel; Hernandez-Benito, Jesus; Calle, Emilio; Casado, Julio

CS Departamento de Quimica Fisica, Universidad de Salamanca, Salamanca, E-37008, Spain

SO Journal of the American Chemical Society (2002), 124(10), 2177-2182 CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English
AB Nitrosa

Nitrosation reactions of amino acids with an -NH2 group (six  $\alpha$ -amino acids: glycine, alanine,  $\alpha$ -aminobutyric acid,  $\alpha$ aminoisobutyric acid, valine, and norvaline; two  $\beta$  amino acids:  $\beta$ -alanine and  $\beta$ -aminobutyric acid; and one  $\gamma$ -amino acid:  $\gamma$ -aminobutyric acid) were studied. Nitrosation was carried out in aqueous acid media, mimicking the conditions of the stomach lumen. The rate equation was  $r = k3 \exp[amino]$ acid] [nitrite] 2, with a maximum k3 exp value in the 2.3-2.7 pH range. existence of an isokinetic relationship supports the argument that all the reactions share a common mechanism. A nitrosation mechanism is proposed, and the following conclusions are drawn: (1) nitrosation reactions of amino acids with a primary amino group in acid media occur with dinitrogen trioxide as the main nitrosating agent. (2) The finding that the nitrosation rate is proportional to the square of the nitrite concentration suggests that the yield of nitrosation products in the stomach would increase sharply with higher nitrate/nitrite intakes. Stomach hypochlorhydria could be a potential enhancer of in vivo amino acid nitrosation. (3) The reactivity (k3 exp) ( $\alpha$ -amino acids > . beta.-amino acids >  $\gamma$ -amino acids) is the same as that found in a previous work for the alkylating potential of lactones formed from nitrosation products of the same amino acids. This implies that the nitrosation reactions of the most common natural amino acids are the most efficient precursors of the most powerful alkylating agents. (4) The order of magnitude (107-108 M-1 s-1) of the bimol. rate consts. of nitrosation shows that such reactions occur through an encounter process.

IT 541-48-0, β-Aminobutyric acid
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical
 process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant

or reagent)

(reactivity of amino acids in nitrosation reactions and its relation to the alkylating potential of their products)

RN 541-48-0 CAPLUS

CN Butanoic acid, 3-amino- (CA INDEX NAME)

NH<sub>2</sub> | Me- CH- CH<sub>2</sub>- CO<sub>2</sub>H

RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2001:331744 CAPLUS

DN 135:15766

TI Basic chemical rule of molecular evolution

AU Zhao, Yu-fen; Lu, Kui

CS Key Laboratory for Bioorganic Phosphorus Chemistry of Ministry of Education, Tsinghua University, Beijing, 100084, Peop. Rep. China

SO Xiamen Daxue Xuebao, Ziran Kexueban (2001), 40(2), 360-365 CODEN: HMHHAF; ISSN: 0438-0479

PB Xiamen Daxue

DT Journal

LA Chinese

AB Peptides and nucleotides could be obtained by self-organizing from N-phosphoryl- $\alpha$ -amino acids in water or organic solvent. However, beta.-amino acids or  $\gamma$ -amino acids could not have the similar reactions in the same conditions. It was found that the characteristics of phosphorus chemical was decided on the characteristics of the mol. structure. The penta-coordinated phosphorus compds. had the single chemical selectivity for  $\alpha$ -amino acids and ribose. The chemical selectivity accelerated the natural selective.

RN 56-84-8 CAPLUS

CN L-Aspartic acid (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

L9 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2001:21346 CAPLUS

DN 134:71895

TI Method for preparation of  $\beta$  -amino acids from amino alcohols

IN Kameyama, Naotaka; Furukawa, Yoshiaki

PA Daiso Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 6 pp. CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI JP 2001002630 A 20010109 JP 1999-168551 19990615

PRAI JP 1999-168551 19990615 CASREACT 134:71895; MARPAT 134:71895 os  $\beta$  -Amino acids represented by formula AB R1CH(NP1P2)CH2CO2H (both P1 and P2 are same or different amino-protecting group; either one of P1 and P2 is amino-protecting group and the other is H) are prepared by introducing a leaving to N-protected amino alc. represented by formula R1CH(NP1P2)CH2OH (P1, P2, R1 = same as above) reaction of the resulting R1CH(NP1P2)CH2X (X = leaving group; P1, P2, R1 = same as above) with a cyanation reagent, and hydrolysis of the resulting nitrile represented by formula R1CH(NP1P2)CH2CN (P1, P2, R1 = same as This process efficiently gives  $\beta$  amino acids in reduced steps, simple procedure, and good yields using readily available raw materials and inexpensive reagents. The  $\beta$  -amino acids are useful as intermediates for  $\beta$ -lactam antibiotics. Thus, 1.04 g methanesulfonyl chloride was added dropwise to a mixture of N-benzyloxycarbonyl-Dphenylalaninol 2.0, Et3N 1.27, 4-dimethylaminopyridine 0.04 g, 20 mL CH2Cl2 under ice-cooling and stirred at 15° for 2 h to give the mesylate (85% yield) which (2.17 g) was stirred with 0.32 g NaCN in 10 mL DMF at 70° for 4 h to give the nitrile (83%). To a mixture of the nitrile (1.45 g) and 4 mL 1,4-dioxane was added 5 mL concentrated 35% HCl and heated with stirring at 90° for 4 h to give, after purification on a column of Amberlite IR120B, 80% (R)-3-amino-4-phenylbutanoic acid. IT 40469-85-0, (S)-3-Amino-4-methylpentanoic acid RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of  $\beta$  -amino acids from amino alcs.) RN 40469-85-0 CAPLUS CN Pentanoic acid, 3-amino-4-methyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

IT 3775-73-3P, (R)-3-Aminobutyric acid 131270-08-1P, (R)-3-Amino-4-phenylbutanoic acid RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of  $\beta$  -amino acids from amino alcs.)

RN 3775-73-3 CAPLUS
CN Butanoic acid, 3-amino-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 131270-08-1 CAPLUS CN Benzenebutanoic acid,  $\beta$ -amino-,  $(\beta R)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

- L9 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN
- AN 2000:442513 CAPLUS
- DN 133:249134
- TI Application of a new chiral stationary phase containing the glycopeptide antibiotic A-40,926 in the direct chromatographic resolution of . beta.-amino acids
- AU D'Acquarica, I.; Gasparrini, F.; Misiti, D.; Zappia, G.; Cimarelli, C.; Palmieri, G.; Carotti, A.; Cellamare, S.; Villani, C.
- CS P. le Aldo Moro 5, Dip. Studi di Chimica e Tecnologia delle Sostanze Biologicamente Attive, Universita 'La Sapienza', Rome, 00185, Italy
- SO Tetrahedron: Asymmetry (2000), 11(11), 2375-2385 CODEN: TASYE3; ISSN: 0957-4166
- PB Elsevier Science Ltd.
- DT Journal
- LA English
- AB A new enantioselective HPLC procedure for the direct resolution of . beta.-amino acids is described, based on the use of a new chiral stationary phase (CSP) containing the macrocyclic glycopeptide antibiotic A-40,926, structurally related to teicoplanin, covalently bonded to silica gel microparticles. The new CSP shows higher enantioselectivity and broader applicability in this field compared to the parent teicoplanin phase. The potential for semi-preparative sepns. on the A-40,926-CSP is demonstrated for a selected cyclic  $\beta$ -amino acid.
- IT 3775-73-3 40469-85-0
  - RL: PEP (Physical, engineering or chemical process); PROC (Process) (application of a new chiral stationary phase containing glycopeptide antibiotic A-40,926 in direct chromatog. resolution of  $\beta$  -amino acids)
- RN 3775-73-3 CAPLUS
- CN Butanoic acid, 3-amino-, (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 40469-85-0 CAPLUS

CN Pentanoic acid, 3-amino-4-methyl-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RE.CNT 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L9 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN
- AN 1999:26278 CAPLUS
- DN 130:162702
- TI Biological and pharmacokinetic studies with  $\beta$ -peptides
- AU Seebach, Dieter; Abele, Stefan; Schreiber, Juerg V.; Martinoni, Bruno; Nussbaum, Alexander K.; Schild, Hansjoerg; Schulz, Henk; Hennecke, Hauke; Woessner, Ralph; Bitsch, Francis
- CS Laboratorium Organische Chemie, Eidgenoessische Technische Hochschule Zurich, Zurich, CH-8092, Switz.
- SO Chimia (1998), 52(12), 734-739 CODEN: CHIMAD; ISSN: 0009-4293

PB Neue Schweizerische Chemische Gesellschaft

DT Journal

LA English

Interactions and cleavage reactions of p-amino acids and  $\beta$ -oligopeptides (up to 9 residues, carrying the side chains of Ala, Val, Leu, Ile, Phe, Ser, Lys, and Hop) with biol. systems, such as the most potent peptidases (pronase, proteinase K, 20S proteasome), microorganisms (Pseudomonas aeruginosa and Pseudomonas putida), and mammalian blood (i.v. application to rats) were investigated and compared with  $\alpha$ -peptides. The results are: i: the 3 peptidases do not cleave  $\beta\text{-peptides}$  at all (within 24 h), and they are not inhibited by a  $\beta$ -peptide; ii: except for certain 3-aminobutanoic-acid ( $\beta$ -HAla) derivs., neither free, nor N-acetyl- $\beta$  -amino acids, nor  $\beta$ -peptides (offered as sole N and C source) lead to growth of the 2 bacteria tested; iii: 2 water-soluble  $\beta$ -heptapeptides (with Lys side chains) were shown to have elimination half-lives  $t1/2(\beta)$  of 3 and 10 h at 100- and 30-ng/mL levels, resp., in the rodent blood - much larger than those of  $\alpha\text{-peptides}$ . Thus, the preliminary results described here confirm the much greater stability of  $\beta$ -peptides, as compared to  $\alpha$ -peptides, towards metabolization processes, but they also suggest that there may be interactions (by hitherto unknown mechanisms) between the worlds of  $\alpha$ - and  $\beta$ -peptides.

IT 3775-72-2 22818-43-5 75946-24-6

75992-50-6

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(biol. and pharmacokinetic studies with  $\beta$ -peptides)

RN 3775-72-2 CAPLUS

CN Butanoic acid, 3-amino-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 22818-43-5 CAPLUS

CN Hexanoic acid, 3-amino-5-methyl-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 75946-24-6 CAPLUS

CN Hexanoic acid, 3-amino-4-methyl-, (3R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 75992-50-6 CAPLUS

CN Pentanoic acid, 3-amino-4-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1995:328908 CAPLUS

DN 122:240416

TI Design of orally active, non-peptide fibrinogen receptor antagonists. An evolutionary process from the RGD sequence to novel antiplatelet aggregation agents

AU Bovy, P. R.; Tjoeng, F. S.; Rico, J. G.; Rogers, T. E.; Lindmark, R. J.; Zablocki, J. A.; Garland, R. B.; McMackins, D. E.; Dayringer, H.; et al.

CS Thrombosis Research, Searle, Skokie, IL, 60077, USA

SO Bioorganic & Medicinal Chemistry (1994), 2(9), 881-95 CODEN: BMECEP; ISSN: 0968-0896

PB Elsevier

DT Journal

LA English

GI

$$H_{2}N$$
 $H_{2}N$ 
 $H_{2$ 

The evolutionary process from the Arg-Gly-Asp-Phe (RGDF) tetrapeptide to potent orally active antiplatelet agents is presented. The RGD sequence is an important component in the recognition of fibrinogen by its platelet receptor GP IIb-IIIa (integrin  $\alpha IIb\beta 3)$ . This work concs. on the replacement of the Arg-Gly dipeptidyl fragment by an acylated aminobenzamidine. The C-terminal fragment has been replaced by a variety of  $\beta$ -amino acids, expanding on a previously reported paradigm. The lead compds. showed good potency in an in vitro platelet aggregation assay (dog PRP/ADP). The affinity for the fibrinogen receptor was confirmed in several cases by the ability to inhibit 235I fibrinogen binding to activated human platelets. The Et ester prodrug form was tested by oral administration to dogs and monitoring of the anti-platelet effect on ex

vivo collagen induced platelet aggregation. From the structural studies reported, the (amidinophenyl) succinamic acid derivative 4- [HN:C(NH2)]C6H4NHCOCH2CH2CO2H was the best surrogate for the Arg-Gly dipeptide. Several conformationally restricted analogs are also reported which are compatible with the hypothesis of RGD binding to the  $\alpha IIb\beta 3$  in a turn-extended-turn conformation. The structure-activity relationships described also underline the importance of the  $\beta$ -amino acid substitution for potency. In particular, the absolute configuration at the  $\beta$ -carbon was crucial for high affinity. The best acid/ester pairs (I and II; R = H, Et) reported in this study had high potency (R = H; PRP/ADP IC50 .simeq. 50 nM) and showed good oral activity in dogs at 5 mg/kg per os (R = Et).

IT 541-48-0,  $(\pm)-3$ -Aminobutyric acid

RL: RCT (Reactant); RACT (Reactant or reagent)
(design and synthesis of orally active nonpeptide fibrinogen receptor antagonists)

RN 541-48-0 CAPLUS

CN Butanoic acid, 3-amino- (CA INDEX NAME)

NH<sub>2</sub> | Me- CH- CH<sub>2</sub>- CO<sub>2</sub>H

L9 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1995:294154 CAPLUS

DN 122:291528

TI Preparation of optically active  $\beta$  -amino acids by asymmetric hydrogenation of (Z)-3-N-acylamino-3-alkylacrylic acids

IN Saburi, Masahiko; Ueda, Yoichiro; Oonishi, Atsushi

PA Daicel Chem, Japan

SO Jpn. Kokai Tokkyo Koho, 21 pp. CODEN: JKXXAF

DT Patent

LA Japanese

FAN CNT 1

GI

FAN.	CNT 1 PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	JP 06271520	Α	19940927	JP 1993-60011	19930319	
	JP 3493206	B2	20040203			
PRAI	JP 1993-60011		19930319			
os	CASREACT 122:291528	; MARPA	AT 122:291528	•		

$$R^4$$
 $R^4$ 
 $R^4$ 

Optically active  $\beta$  -amino acids

R1CONHCHR2CH2CO2H (R1 = lower alkyl, Ph, CH2Ph; R2 = lower alkyl, optionally substituted by Ph or alkoxycarbonyl), useful as intermediates for physiol. active peptides or  $\beta$ -lactam antibiotics, are prepared by asym. hydrogenation of (Z)-3-N-acylamino-3-alkylacrylic acids <math>(I; R1, R2 =same as above) in the presence of an optically active ruthenium-phosphine complex, particularly represented by RuHCl(R4-BINAP)2, [RuH(R4-BINAP)2]Y, or [Ru(R4-BINAP)] (O2CR5)2 (wherein R4-BINAP is represented by tertiary phosphine II; R4 = H, lower alkyl; Y = BF4-, PF6-, ClO4-, SbF6-; R5 = lower alkyl). This process uses relatively inexpensive catalysts, ruthenium-phosphine complexes, and gives  $\beta$  amino acids of high optical purity. Thus, 58 mg (Z)-3-benzamido-2-hexenoic acid (III), 3.7 mg [RuH[(+)-BINAP]]2PF6 (preparation given), 1.25 mL THF, and 1.25 mL MeOH were hydrogenated in a stainless steel autoclave under H pressure 5 atm at 50° for 24 h to give 100% (3S)-(+)-3-benzamidohexanoic acid of 83% e.e. Similarly, asym. hydrogenation of III in the presence of [Ru[(-)-BINAP]](O2CCMe3)2 (preparation given) gave 100% (3R)-(-)-3-benzamidohexanoic acid of 72% e.e. IT 26250-87-3P, (3S)-(+)-3-Amino-4-phenylbutyric acid 40469-85-0P, (3S)-(+)-3-Amino-4-methylpentanoic acid 75992-50-6P, (3R)-(-)-3-Amino-4-methylpentanoic acid 91298-66-7P, (3S)-(+)-3-Aminohexanoic acid 131270-08-1P, (3R)-(-)-3-Amino-4-phenylbutyric acid RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of optically active  $\beta$  -amino acids by asym. hydrogenation of (Z)-3-N-acylamino-3alkylacrylic acids) RN 26250-87-3 CAPLUS Benzenebutanoic acid,  $\beta$ -amino-,  $(\beta S)$ - (9CI)(CA INDEX NAME)

Absolute stereochemistry.

AB

RN 40469-85-0 CAPLUS CN Pentanoic acid, 3-amino-4-methyl-, (3S)- (CA INDEX NAME) Absolute stereochemistry. Rotation (+).

RN 75992-50-6 CAPLUS

CN Pentanoic acid, 3-amino-4-methyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 91298-66-7 CAPLUS

CN Hexanoic acid, 3-amino-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 131270-08-1 CAPLUS

CN Benzenebutanoic acid,  $\beta$ -amino-,  $(\beta R)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$HO_2C$$
  $R$   $Ph$   $NH_2$ 

- L9 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN
- AN 1995:30133 CAPLUS
- DN 122:106415
- TI Biocatalytic resolution of  $\beta$ -fluoroalkyl-  $\beta$  -amino acids
- AU Soloshonok, Vadim A.; Kirilenko, Alexander G.; Fokina, Nataly A.; Shishkina, Irine P.; Galushko, Sergey V.; Kukhar, Valery P.; Svedas, Vytas K.; Kozlova, Elena V.
- CS Catalysis Res. Center, Hokkaido Univ., Sapproro, 060, Japan
- SO Tetrahedron: Asymmetry (1994), 5(6), 1119-26 CODEN: TASYE3; ISSN: 0957-4166
- DT Journal
- LA English
- OS CASREACT 122:106415

GI

AB Racemic N-phenylacetyl- $\beta$ -fluoroalkyl- $\beta$ -alanines ( $\pm$ )-I (R = CF3, C2F5, C3F7, CHF2) were synthesized and biocatalytically resolved to the corresponding enantiopure  $\boldsymbol{\beta}$  -amino acids II and III with the aid of penicillin acylase (EC 3.5.1.11) from Escherichia coli. In substrates (±)-I the enantioselectivity of the biocatalytic process was practically uninfluenced by the nature of the fluoroalkyl chain. Thus,  $\beta$ -fluoroalkyl- $\beta$ -alanines II and II bearing short or long chains were prepared in high enantiomeric purity. The (R)-enantiomer was the fast-reacting enantiomer in all cases. IT 584-20-3 77162-46-0 150618-42-1 150618-43-2 160707-31-3 178381-12-9 RL: RCT (Reactant); RACT (Reactant or reagent) (acylation of, with phenylacetyl chloride) RN 584-20-3 CAPLUS

CN Butanoic acid, 3-amino-4,4,4-trifluoro- (9CI) (CA INDEX NAME)

$$^{
m NH}_{
m 2}$$
  $^{
m |}$   $^{
m F}_{
m 3}$ C- CH- CH $_{
m 2}$ - CO $_{
m 2}$ H

RN 77162-46-0 CAPLUS CN Butanoic acid, 3-amino-4,4-difluoro- (9CI) (CA INDEX NAME)

$$\begin{array}{c} ^{\rm NH_2} \\ | \\ {\rm F_2CH-CH-CH_2-CO_2H} \end{array}$$

RN 150618-42-1 CAPLUS CN Hexanoic acid, 3-amino-4,4,5,5,6,6,6-heptafluoro- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NH}_2 \\ | \\ \text{HO}_2\text{C--} \text{CH}_2\text{--} \text{CH---} \text{CF}_2\text{---} \text{CF}_3 \end{array}$$

RN 150618-43-2 CAPLUS CN Pentanoic acid, 3-amino-4,4,5,5,5-pentafluoro- (9CI) (CA INDEX NAME)

RN 160707-31-3 CAPLUS CN Heptanoic acid, 3-amino-4,4,5,5,6,6,7,7-octafluoro- (9CI) (CA INDEX NAME)

RN 178381-12-9 CAPLUS

CN Pentanoic acid, 3-amino-4,4,5,5-tetrafluoro- (9CI) (CA INDEX NAME)

IT 109537-89-5P 111218-68-9P 151871-99-7P 151911-19-2P 151911-20-5P 151911-21-6P

151911-30-7P 151911-31-8P 157201-07-5P

157201-08-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, via biocatalytic resolution)

RN 109537-89-5 CAPLUS

CN Butanoic acid, 3-amino-4,4-difluoro-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 111218-68-9 CAPLUS

CN Butanoic acid, 3-amino-4,4-difluoro-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 151871-99-7 CAPLUS

CN Butanoic acid, 3-amino-4,4,4-trifluoro-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 151911-19-2 CAPLUS

CN Butanoic acid, 3-amino-4,4,4-trifluoro-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 151911-20-5 CAPLUS

CN Pentanoic acid, 3-amino-4,4,5,5,5-pentafluoro-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 151911-21-6 CAPLUS

CN Hexanoic acid, 3-amino-4,4,5,5,6,6,6-heptafluoro-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 151911-30-7 CAPLUS

CN Pentanoic acid, 3-amino-4,4,5,5,5-pentafluoro-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 151911-31-8 CAPLUS

CN Hexanoic acid, 3-amino-4,4,5,5,6,6,6-heptafluoro-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 157201-07-5 CAPLUS

CN Pentanoic acid, 3-amino-4,4,5,5-tetrafluoro-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 157201-08-6 CAPLUS

CN Heptanoic acid, 3-amino-4,4,5,5,6,6,7,7-octafluoro-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L9 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1994:320016 CAPLUS

DN 120:320016

TI Osmotic regulation of taurine transport via system  $\beta$  and novel processes in mouse preimplantation conceptuses

AU Van Winkle, Lon J.; Patel, Meghana; Wasserlauf, Howard G.; Dickinson, Helen R.; Campione, Allan L.

CS Department of Biochemistry,, Midwestern University, Downers Grove, IL, 60515, USA

SO Biochimica et Biophysica Acta, Biomembranes (1994), 1191(2), 244-55 CODEN: BBBMBS; ISSN: 0005-2736

PB Elsevier B.V.

DT Journal

LA English

The authors studied transport of taurine and related amino acids by AB preimplantation mouse conceptuses. The most conspicuous component of taurine transport in conceptuses at the 1-cell through blastocyst stages of development was both Na+ and Cl- dependent. This Na+- and Cl--dependent transport system interacted relatively strongly with  $\beta$ but not  $\alpha\text{-amino}$  acids. By these criteria, transport system  $\beta$ is responsible for Na+-dependent taurine transport in preimplantation mouse conceptuses. Moreover, detection of mRNA encoding the taurine transport protein (TAUT) in early conceptuses supports the theory that TAUT is a major component of system  $\beta$ . Transport of taurine by system  $\beta$  in 1-cell conceptuses was slower in hypotonic than in hypertonic media, whereas the reverse was true for system  $\beta$  in blastocysts. In contrast, hypotonically stimulated Na+-independent taurine transport was, of course, more rapid in hypotonic than in hypertonic media in both 1-cell conceptuses and blastocysts. Transport via this hypotonically stimulated process also showed no sign of saturation by up to 10 mM taurine. Hypotonically stimulated taurine transport appeared transiently in 1-cell conceptuses under hypotonic conditions until they had recovered their initial vols. Hence, the authors suggest that a decrease in taurine uptake via system  $\beta$  and an increase in taurine exodus via the Na+-independent, nonsaturable transport process could contribute to the regulatory volume decrease in 1-cell conceptuses in hypotonic medium. Since taurine uptake by system  $\beta$  in blastocysts is, however, higher in hypotonic than in hypertonic media, taurine uptake by system  $\beta$  in blastocysts might intensify a tendency to increase cell volume in hypotonic medium. Such an increase in taurine uptake could further favor anabolic changes associated with cell swelling. In addition to contributing to regulation of cellular volume and perhaps metabolism, the hypotonically stimulated Na+-independent transport

processes in early embryos have novel characteristics. Hypotonically stimulated Na+-independent taurine transport was inhibited by niflumate, N-ethylmaleimide, and NaN3 but not by furosemide, iodoacetate, KCN, ouabain, or  $\alpha$ - or  $\beta$  -amino acids. Furthermore, DIDS inhibited this transport in 1-cell conceptuses but not in blastocysts. Hence, different hypotonically stimulated Na+-independent taurine transport processes appear to be present in 1-cell conceptuses vs. blastocysts. The functions of these and other instances of developmental regulation of expression of transport processes in preimplantation conceptuses remain largely to be elucidated. Moreover, neither of the hypotonically stimulated Na+-independent taurine transport processes in conceptuses appears to have been detected in other types of cells. Instead, these processes may be unique to preimplantation conceptuses.

56-84-8, Aspartic acid, biological studies IT

RL: BIOL (Biological study)

(transport of, by preimplantation embryo, regulation of)

56-84-8 CAPLUS RN

L-Aspartic acid (CA INDEX NAME) CN

Absolute stereochemistry. Rotation (+).

L9 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN

1994:266834 CAPLUS ΑN

120:266834 DN

Properties of osmolyte fluxes activated during regulatory volume decrease TI in cultured cerebellar granule neurons

ΑU Pasantes-Morales, H.; Chacon, E.; Murray, R. A.; Moran, J.

CS Inst. Cell Physiol., Natl. Univ. Mexico, Mexico City, Mex.

SO Journal of Neuroscience Research (1994), 37(6), 720-7 CODEN: JNREDK; ISSN: 0360-4012

DT Journal

English LΑ

Efflux pathways for amino acids, K, and Cl activated during regulatory AB volume decrease (RVD) were characterized in cultured cerebellar granule neurons exposed to hyposmotic conditions. Results of this study favor diffusion pores (presumably channels) over energy-dependent transporters as the mechanisms responsible for the efflux of these osmolytes. The selectivity of osmolyte pathways activated by RVD was assessed by increasing the extracellular concns. of cations, anions, and amino acids to such an extent that upon opening of the pathway, a permeable compound will enter the cell and block RVD by reducing the efflux of water carried by the exit of intracellular osmolytes. The cationic pathway was found selective for K (and Rb), whereas the anionic pathway was rather unselective being permeable to Cl, nitrate, iodine, benzoate, thiocyanate, and sulfate but impermeable to gluconate. Glutamate and aspartate as K but not as Na salts were permeable through the anion channel. RVD was slightly inhibited by quinidine but otherwise was insensitive to known K channel blockers. RVD was inhibited by DIDS, niflumic acid, and dipyridamole. Gramicidin did not affect cell volume in isosmotic conditions but greatly accelerated RVD, suggesting that cell permeability to Cl is low in isosmotic conditions but increases markedly during RVD making K permeability the rate limit of the process. The permeability pathway for amino acids activated during RVD was permeable to short chain  $\alpha$ - and  $\beta$  -amino acids, but excluded glutamine and basic amino acids.

IT 56-84-8, Aspartic acid, biological studies 14007-45-5,

Potassium aspartate 17090-93-6, Sodium aspartate

RL: BIOL (Biological study)

(transport of, by brain cerebellar granule in regulatory volume decrease)

RN 56-84-8 CAPLUS

CN L-Aspartic acid (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 14007-45-5 CAPLUS

CN L-Aspartic acid, potassium salt (1:?) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

●x K

RN 17090-93-6 CAPLUS

CN L-Aspartic acid, sodium salt (1:?) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

●x Na

L9 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1991:628003 CAPLUS

DN 115:228003

TI Distribution of compatible solutes in the halophilic methanogenic archaebacteria

AU Lai, Mei Chin; Sowers, Kevin R.; Robertson, Diane E.; Roberts, Mary F.; Gunsalus, Robert P.

CS Dep. Microbiol. Mol. Genet., Univ. California, Los Angeles, CA, 90024, USA

SO Journal of Bacteriology (1991), 173(17), 5352-8 CODEN: JOBAAY; ISSN: 0021-9193

DT Journal

LA English

AB Accumulation of compatible solutes, by uptake or de novo synthesis, enables bacteria to reduce the difference between osmotic potentials of the cell cytoplasm and the extracellular environment. To examine this process in the halophilic and halotolerant methanogenic archaebacteria, 14 strains were tested for the accumulation of compatible solutes in response to growth in various extracellular concns. of NaCl. In external NaCl concns. of 0.7-3.4M, the halophilic methanogens accumulated K+ and low-mol.-weight organic compds. β-Glutamate was detected in two halotolerant strains that grew below 1.5 NaCl. Two

unusual  $\beta$  -amino acids, Ne-acetyl- $\beta$ -lysine and  $\beta$ -glutamine (3-aminoglutaramic acid), as well as L- $\alpha$ -glutamate were compatible solutes among all of these strains. De novo synthesis of glycine betaine was also detected in several strains of moderately and extremely halophilic methanogens. The zwitterionic compds. ( $\beta$ -glutamine, Ne-acetyl- $\beta$ -lysine, and glycine betaine) and K were the predominant compatible solutes among the moderately and extremely halophilic methanogens. This is the first report of  $\beta$ -glutamine as a compatible solute and de novo biosynthesis of glycine betaine in the methanogenic archaebacteria.

IT 1948-48-7 6706-21-4,  $\beta$ -Glutamine

131887-44-0

RL: BIOL (Biological study)

(osmotic potential adaptation in halophilic methanogenic archaebacteria in relation to accumulation of)

RN 1948-48-7 CAPLUS

CN Pentanedioic acid, 3-amino- (CA INDEX NAME)

$$\begin{array}{c} {\rm NH_2} \\ | \\ {\rm HO_2C-CH_2-CH-CH_2-CO_2H} \end{array}$$

RN 6706-21-4 CAPLUS

CN Pentanoic acid, 3,5-diamino-5-oxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{NH}_2 & \text{O} \\ & | & || \\ \text{HO}_2\text{C}-\text{CH}_2-\text{CH}-\text{CH}_2-\text{C}-\text{NH}_2 \end{array}$$

RN 131887-44-0 CAPLUS

CN Hexanoic acid, 6-(acetylamino)-3-amino- (9CI) (CA INDEX NAME)

$$^{\mathrm{NH}_{2}}_{|}$$
 $_{\mathrm{HO}_{2}\mathrm{C}^{-}\,\mathrm{CH}_{2}^{-}\,\mathrm{CH}^{-}\,(\mathrm{CH}_{2})_{\,3}^{\,-}\,\mathrm{NHAc}}$ 

L9 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN

AN . 1953:12476 CAPLUS

DN 47:12476

OREF 47:2234g-i

TI Isolation and amino acid composition of  $\beta$ -globulin extracted from the seeds of barley (Hordeum vulgare)

AU Jensen, Robert

CS Carlsberg Breweries, Copenhagen

SO Acta Chemica Scandinavica (1952), 6, 771-81 CODEN: ACHSE7; ISSN: 0904-213X

DT Journal

LA English

AB The β-globulin was prepared by extracting ground barley with N NaCl and precipitating by 15% saturation with (NH4)2SO4; this process was repeated 4 times and the product dialyzed. The diffusion constant is 4.8 when calculated by the area method and 4.9 + 10-7 cm.2/sec. by the "second moment" method. The electrophoretic mobility is 3.5 + 10-5 cm.2/v./sec. at pH 7.05 and the peak is homogeneous throughout the determination The sedimentation constant in 0.2 N NaCl at 24° is 6.7. After hydrolysis the amino acids were separated by starch chromatography and quantitatively determined (Moore and Stein (C.A. 43, 5818d)). Corrected values (reported as % N of total N) are: leucine 7.3; isoleucine 2.1; phenylalanine 2.5;

methionine 1.9; valine 7.1; tyrosine 4.1; proline 10.1; glutamic acid 10.6; alanine 6.4; threonine 4.3; aspartic acid 5.8; serine 3.6; glycine 4.9; NH3 11.8; arginine 5.4; lysine 2.5; histidine 2.8; cystine and cysteine 6.8. Tryptophan constituted 3.8% of the protein weight.

IT 56-84-8, Aspartic acid

(in  $\beta$ -globulin from barley)

RN 56-84-8 CAPLUS

CN L-Aspartic acid (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

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Society, Washington, D. C.

CODEN: 69IHRD

- DT Conference; Meeting Abstract; (computer optical disk)
- LA English
- AB The chemical of poly(beta-aminoacids) has been experiencing a renaissance in recent years due to the ability of these materials to mimic secondary structural features of peptides. They have found application as peptide mimetics in pharmaceuticals, anti-microbial surfaces and medicinal applications where they are particularly valued due to their resistance to peptidases and other hydrolytic enzymes. The single-step synthesis of these polymers, via the metal catalyzed ring opening polymerization of lactams is presented. The synthesis and characteriation of well defined yttrium(III) amide complexes are described and these species are highly active and controlled catalysts for the ring opening polymerization of (S)-4-(Benzyloxylcaronyl)-2-azetidone. The polymerization kinetics and mechanism are studied and the catalysts are shown

exert good polymerization control. The catalysts are also active for the ring opening polymerization of lactones and can be used to synthesize novel block copoly(ester-amides).

- L2 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
- AN 2006:693765 CAPLUS
- DN 145:315252

to

- TI A solution to the component instability problem in the preparation of peptides containing C2-substituted cis-cyclobutane  $\beta$  aminoacids: synthesis of a stable rhodopeptin analog
- AU Roy, Olivier; Faure, Sophie; Aitken, David J.
- CS Laboratoire SEESIB-CNRS, Departement de Chimie, Universite Blaise Pascal, Clermont-Ferrand II, Aubiere, 63177, Fr.
- SO Tetrahedron Letters (2006), 47(33), 5981-5984 CODEN: TELEAY; ISSN: 0040-4039
- PB Elsevier B.V.
- DT Journal
- LA English
- OS CASREACT 145:315252
- AB Despite the inherent instability of C2-substituted cis-cyclobutane . beta.-aminoacids, incorporation of such residues into peptides is shown to be possible through use of a 1-amino-2- (hydroxymethyl)cyclobutane derivative as a stable  $\beta$ -aminoacid surrogate. This synthetic strategy was validated by the synthesis of a rhodopeptin analog.
- RE.CNT 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L2 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
- AN 2005:124735 CAPLUS
- TI Enzymatic resolution of cyclic N-Boc protected  $\beta$  aminoacids [Tetrahedron: Asymmetry 15 (2004) 3407]
- AU Pousset, Cyrille; Callens, Roland; Haddad, Mansour; Larcheveque, Marc
- CS Laboratoire de Synthese Organique, ENSCP, CNRS, Paris, 75231 05, Fr.
- SO Tetrahedron: Asymmetry (2005), 16(3), 745 CODEN: TASYE3; ISSN: 0957-4166
- PB Elsevier B.V.
- DT Journal; Errata
- LA English
- AB Unavailable
- L2 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
- AN 2003:522188 CAPLUS
- TI Solution NMR and x-ray crystal structures of new chiral 1,4-oxazepinium heterocycles from 2,4-pentanedione
- AU Lozada, Concepcion
- CS Instituto de Quimica, UNAM, Coyo, Mex.
- SO Abstracts, 36th Middle Atlantic Regional Meeting of the American Chemical Society, Princeton, NJ, United States, June 8-11 (2003), 319 Publisher: American Chemical Society, Washington, D. C.

CODEN: 69EBDT

DT Conference; Meeting Abstract

LA English

AB The reaction of 2,4-pentanedione 1 with (R)-(-)-2-phenylglycine Me ester 2, (R)-(-)-2-phenylglycinol 3 and the proteinogenic aminoacids (2S, 3R) (-)-2-amino-3-hydroxybutyric acid (L-Threonine) 4, and (R)-(-)-2-amino-3-mercaptopropionic acid (L-cysteine) 5 Me esters was investigated. The corresponding enamines 6, 7, 8 were isolated and characterized spectroscopically while 9, unstable, was transformed in situ into 13. Furthermore, treatment of 7, 8 and 9 with Boron trifluoride etherate, afforded the new [1,4] oxazepines 10, 11, and [1,4] thiazepine 12 as their BF30- salts. The structure of enamines and their corresponding seven member heterocycles was assessed by 1D and 2D NMR spectroscopy and by X-ray crystalog. detns. Variable temperature expts. showed different mol. mobility among these heterocycles. As a part of our studies with  $\beta\text{-diketone}$  compds. of natural origin, it became necessary to explore the reactivity of this chemical functionality with some  $\alpha\text{-L-amino}$  acid Me esters and other chiral compds. i.e. (R)-(-)-2-phenylglycinol. Such reactions have led at a first step to the corresponding enamines; resulted from the nucleophilic attack of the primary amine function to 2,4-pentanedione at room temperature in CH2Cl2, with Me esters of  $\beta$  -aminoacids. Resulting products further were transformed into the corresponding seven-membered heterocycles, upon treatment with boron trifluoride etherate at room temperature

The NMR spectra of these heterocycles are distinct and uniquely associated with each of these structures.

L2 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1906:103540 CAPLUS

DN 0:103540

TI Synthesis of thymine and other uracils

AU Fischer, Emil; Roeder, George

SO Sitzungsberichte der Akademie der Wissenschaften in Berlin (1901), 12, 268-76

From: J. Chem. Soc., Abstr. 80, I, 294-5 1901

CODEN: SAWBEB

DT Journal

LA Unavailable

AB Hydrouracils may be produced either by the interaction of potassium cyanate and the salts of the esters of  $\beta$ -aminoacids , or by heating carbamide with an unsaturated acid. The preparations of 4-methyldihydrouracil, ethyl  $\beta$ -aminobutyrate, bromo-4-methyldihydrouracil, methyluracil, and 5-methyldihydrouracil are discussed. Their characteristics are also described.

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